Dr. MUTHU SANKAR AATHI
Assistant Professor,
Department of Medical Biotechnology,
School of Engineering,
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Google Scholar Link: https://scholar.google.com/citations?user=fHFssx8AAAAJ&hl=en

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Teaching & Research: Looking for a challenging teaching and research position in the field of biotechnology and bioinformatics. I have been working in the field of bioinformatics for more than 12 years. All of my research work focuses on computational structural biology to develop accurate prediction with help of improve the experimental techniques. My research spans across several different areas involving genomics, computer-aided drug design, proteomics, phyloinformatics, network analysis, pharmacophore modeling, quantitative structure-activity relationship, molecular dynamics simulations, small molecule validations and crystallography.

TEACHING EXPERIENCE:

July 2021 – Till date : Assistant Professor,
Department of Biotechnology,
School of Engineering,
Ajeenkya DY Patil University, Pune, India.

EDUCATIONS:

Course	Institution	Year
Ph.D., (Bioinformatics)	Bharathiar University, Coimbatore	2010-2016
M.Phil., (Bioinformatics)	Bharathiar University, Coimbatore	2008-2010
M.Sc., (Bioinformatics)	Bharathiar University, Coimbatore	2006-2008
M.Sc., (Zoology)*	Bharathiar University, Coimbatore	2012-2014
B.Sc., (Zoology)	Manonmaniam Sundaranar University, Tirunelveli	2003-2006

***SDE=School of distance education

RESEARCH EXPERIENCE:

December 2018 – December 2020: ICMR-Post Doctoral Fellow – Dr. Susan Thomas
Biomedical Informatics Centre,
ICMR-National Institute for Research in Reproductive Health (ICMR-NIRRH), Mumbai, India.

Research Title : Discovery validation and structural characterization of therapeutic modulators of human follicle stimulating hormone receptor.

August 2016 – July 2018 National Post Doctoral Fellow–Dr. Arockiasamy Arulandu
Membrane Protein Biology Group,
International Centre for Genetic Engineering and Biotechnology (ICGEB), New Delhi, India.

Research title : Comparative structure-function studies on plant dehydroascorbate reductases (DHARs) and human chloride intracellular channels (hCLICs) that are dimorphic and exist both in soluble and membrane integrated ion-channel forms.

November 2012-November 2015 : UGC-Project Fellow,
DBT-Bioinformatics Centre,
Computational Biology Lab,
Department of Bioinformatics,
Bharathiar University, Coimbatore, Tamil Nadu.

Project Title Computational identification of promoter regions in fungal genomics.

HONORS AND AWARDS:

- ICMR-Post Doctoral Fellow – National Institute for Research in Reproductive Health (ICMR-NIRRH) at Mumbai (December 2018 – December 2020).
- UGC-DS Kothari Post Doctoral Fellow (Selected December 2018 but not availed) - Jawaharlal Nehru University at New Delhi.
- DST-National Post Doctoral Fellow - International Centre for Genetic Engineering and Biotechnology (ICGEB) at New Delhi (August 2016 – July 2018).
- UGC-Project Fellow - DBT-Bioinformatics Centre, Bharathiar University, Coimbatore (November 2012 – November 2015).

- DBT-Traineeship - DBT-Bioinformatics Centre, Bharathiar University, Coimbatore (January 2011 – September 2011).

BIOINFORMATICS SKILLS:

- Expressed Sequence Tag analysis: CAP3 server, ESTScan
- Single Nucleotide Polymorphism analysis: SIFT, PolyPhen
- Protein functional analysis: ScanProsite, Interpro Scan
- Evolutionary analysis : MEGA, CLC Genomics Workbench
- Network analysis : Cytoscape, STRING
- Molecular modeling : Modeller, I-TASSER, Prime (Schrodinger Package)
- Protein structure validation: PROCHECK, Molprobity
- Active site prediction : CASTp, Qsite, COACH
- Screening Libraries : FDA, DrugBank, NCI, Peptidomimetics, PubChem, ZINC
- Draw small molecule : ChemSketch, ChemDraw
- Pharmacokinetics : SwissADME, pkCSM
- Protein-ligand docking: AutoDock, Glide, CDOCKER
- DNA-ligand docking : PatchDock server
- High-throughput virtual screening: Raccoon-AutoDock, AutoDock Vina, Schrodinger, LibDock, GOLD
- Protein-protein docking: ZDOCK
- Molecular dynamics Simulation: Gromacs (protein-ligand, membrane), Desmond
- Molecular visualization: PyMol, RasMol, Chimera, Discovery Studio visualizer, Schrodinger visualizer
- Pharmacophore modeling: Discovery studio, e-pharmacophore (Schrodinger)
- QSAR : Discovery studio, AutoQSAR (Schrodinger)

COMPUTER SKILLS:

- Operating Systems : Windows, LINUX
- Multimedia : Photoshop

EXPERIMENTAL SKILLS (BASIC):

- Mammalian cell culture
- Cloning
- Small molecule validation: Surface Plasmon Resonance
- Co-crystallization

STRUCTURE DETERMINATION (BASIC):

- Crystallography : Coot, Phenix, CCP4, iMosflm

LIST OF PUBLICATIONS:

1. Akanksha Tomar, Sibasis Sahoo, **Muthusankar Aathi**, Shobhan Kuila, Mohd Azeem Khan, Guru Raj Rao Ravi, Jeyakanthan Jeyaraman, Jawahar L Mehta, Kottayil I Varughese, Arockiasamy Arulanadu (2022). Exploring the druggability of oxidized low-density lipoprotein (ox-LDL) receptor, LOX-1, a proatherogenic drug target involved in atherosclerosis. Biochemical and Biophysical Research Communications. 623; 59-65.

https://doi.org/10.1016/j.bbrc.2022.07.036, Publisher: Elsevier

2. **Muthu Sankar Aathi,** Chandan Kumar, Kaushiki S. Prabhudesai, Dhivya Shanmugarajan, Susan Idicula-Thomas (2022). Mapping of FSHR agonists and antagonists binding sites to identify potential peptidomimetic modulators. Biochimica et Biophysica Acta – Biomembranes. 1864: 1-10.

DOI: doi.org/10.1016/j.bbamem.2021.183842, Publisher: Elsevier.

3. G Sathya Priyadarshini, **Aathi Muthusankar**, Ramesh subramani, Selvi Gopal, (2021). Evaluation of the synthesized novel Iridium (III) complexes against HeLa cell lines through *in-silico*, *in-vitro* and DNA nicking. Asian Pacific Journal of Cancer Prevention. 22(2), pp.447-455.

DOI: 10.31557/APJCP.2021.22.2.447, Publisher: Asian Pacific Organization for Cancer Prevention.

4. Kaushiki S Prabhudesai, **Muthu Sankar Aathi**, Vikas Dighe, Susan Idicula-Thomas (2021). A 5-mer peptide derived from hinge region of hFSHR exhibits partial agonist activity *in vivo*. Biochimica et Biophysica Acta – Biomembranes. 1863(1): 1-11.

DOI: 10.1016/j.bbamem.2020.183492, Publisher: Elsevier

7. Arockiasamy Arulanadu, Akanksha Tomar, Azeem Khan, Sibasis Sahoo, **Muthu Sankar Aathi**, Anmol Chandele, Jawahar L Mehta, Kottayil I Varughese (2021). Structure guided inhibitor discovery targeting a membrane receptor involved atherosclerosis. Acta Crystallographica Section A: Foundations and Advances. 77, C39.

8. Ramachandran Srinivasan, Amballa Chaitanyakumar, Parthiban Subramanian, Anbazhagan Mageswari, Ajitha Gomathi, Velmurugan Aswini, **Aathi Muthu Sankar**, Mohandass Ramya, Kodiveri Muthukaliannan Gothandam (2020). Recombinant engineered phage-derived enzybiotic in Pichia pastoris X-33 as whole cell biocatalyst

for effective biocontrol of *Vibrio parahaemolyticus* in aquaculture. International Journal of Biological Macromolecules. 154: 1576-1585.
DOI: 10.1016/j.ijbiomac.2019.11.042, Publisher: Elsevier

9. **Muthusankar Aathi** and Shanmughavel Piramanayagam (2019). From EST to structure models for functional inference of APP, BACE1, PSEN1, PSEN2 genes. Bioinformation. 15(10): 760-771.
DOI: 10.6026/97320630015760, Publisher: Biomedical Informatics

10. Rajendran Satheeshkumar, Lincy Edatt, **Aathi Muthusankar**, V. B. Sameer Kumar and Karnam Jayarampillai Rajendra Prasad (2019). Synthesis of novel quin[1,2-b]acridines: *In vitro* cytotoxicity and molecular docking studies. Polycyclic Aromatic Compounds. 41; 1-15.
DOI: 10.1080/10406638.2019.1689515, Publisher: Taylor and Francis Ltd.

11. Rajendran Satheeshkumar, **Aathi Muthusankar**, Lincy Edatt, V. B. Sameer Kumar, Hazel A. Sparkes and Karnam Jayarampillai Rajendra Prasad (2018). Synthesis of heteroannulated cyclopent[b]indoles: Exploration of *in vitro* cytotoxicity and molecular docking studies. Synthetic Communications. 48: 447-461.
DOI: 10.1080/00397911.2017.1407792, Publisher: Taylor and Francis Ltd.

12. Radhika Ramachandran, **Muthusankar Aathi**, Durairaj D Ruban, Shanmughavel Piramanyagam (2017). Computational Screening of CCR5 Inhibitors as Potential Entry Inhibitor Microbicides Using 3D-QSAR Studies, Docking and Molecular Dynamics Simulation. Current HIV Research. 15; 234-244.
DOI: 10.2174/1570162X15666170106124216, Publisher: Bentham Science

13. Pushparaj Karthika, Chithravel Vadivalagan, **Aathi Muthusankar**, Kadarkarai Murugan, Natraj Krishnaveni, Paola Del Serrone, Marcello Nicoletti, Giovanni Benelli (2017). Methyl linolenate as a feeding stimulant for the 28-spotted potato ladybird, Henosepilachna vigintioctopunctata? A molecular docking approach. Physiological and Molecular Plant Pathology. 101: 75-84.
DOI: 10.1016/j.pmpp.2017.01.005, Publisher: Elsevier

14. Palanivelu Nithya, Sannasi Helena, Jim Simpson, Malaichamy Ilanchelian, **Aathi Muthusankar**, Subbiah Govindarajan (2016). New cobalt(II) and nickel(II) complexes of benzyl carbazate Schiff bases:Syntheses, crystal structures, in vitro DNA and HSA binding studies. Journal of Photochemistry & Photobiology, B: Biology. 165; 220-231.
DOI: 10.1016/J.JPHOTOBIOL.2016.10.024, Publisher: Elsevier

15. Rajendran Selvakumar, Steven J.Geib, **Aathi Muthu Sankar**, Thathan Premkumar, Subbaiah Govindarajan (2015). The chemistry of aminoguanidine derivatives-preparation, crystal structure, thermal properties and molecular docking studies of aminoguanidinium salts of several carboxylic acids. Journal of Physical and Chemistry of Solids. 86; 49-56.
DOI: 10.1016/j.jpcs.2015.05.024, Publisher: Elsevier

16. R. Satheeshkumar, C. Kavitha, **A. Muthusankar**, P. Shanmughavel and K.J. Rajendra Prasad (2015). Quinoline alkaloids – Synthesis, molecular docking studies of atanine, 2-isopropylfuro [2,3-b] quinolines and 3,4-dihydro-2,2-dimethyl-2H-pyrano [2,3-b]quinolines. Indian Journal of Chemistry-B. 54B; 988-998.
DOI: 10.1002/chin.201549170, Publisher: Indian Journal of Chemistry -Section B.

17. K Satyavani, S Gurudeeban, T Ramanathan and **A Muthusankar** (2015). Influence of Rhizophora apiculata Flavonoids on chemical and thermal induced nociceptive models. British Journal of Pharmaceutical Research. v7(2):p102-109.
DOI: 10.9734/BJPR/2015/16732.

18. **Aathi Muthusankar** and Shanmughavel Piramanyagam (2013). *In silico* validation of Human NDRG2 protein against Alzheimer's disease using molecular modeling, docking and dynamics studies. Drug Invention Today. 5; 22-27.
DOI: 10.1016/j.dit.2013.02.002, Publisher: Elsevier

19. Thangavel Indumathi, **Aathi Muthusankar**, Piramanyagam Shanmughavel and KJ Rajendra Prasad (2013). Synthesis of hetero annulated carbazoles; Exploration of *in vitro* cytotoxicity and molecular docking studies. Medicinal Chemistry Communication. v (4); 450-55.
DOI: 10.1039/C2MD20335A, Publisher: Royal Society of Chemistry

20. Lisina K.V, Gopalakrishnan V.K, **Muthusankar Aathi**, Murugesh E and Shanmughavel P (2012). *Insilico* Analysis of Biochemical compounds used as Hepato protective agents. International Journal of Current Research. V4 (6); p30-35.

21. Sathish Kumar R, **Muthusankar Aathi** and Shanmughavel P (2012). A structural insight towards identify specific epitopes of phytoplasma diseases. International Journal of Pharmacy and Biological Sciences. V2 (1); p99-109.

22. **Aathi Muthu Sankar** and P Shanmughavel (2010) *In Silico* Docking Analysis for Viral protein - Hemagglutinin-Neuraminidase against the Synthetic Drugs for Human Parainfluenza virus3. An International Journal of Pharma and Bio Sciences. V1(2); p1-12.

POSTER PRESENTATION AND ABSTRACT PUBLISHED:

- Love Panchariya, Shobhan Kuila, **Muthusankar Aathi**, Arichita Ghoshal, Jeyakanthan Jeyaraman and Arockiasamy Arulandu (2020). Target validation and discovery of anti-cancer therapeutics targeting soluble human chloride intracellular channels. International Conference on Drug Discovery 2020, Hyderabad, India.
- Shobhan Kuila, **Muthusankar Aathi**, Akanksha Tomar, J. Jeyakanthan and Arockiasamy Arulandu (2018). Targeting Chloride Intracellular Channels (CLICs) for anticancer inhibitor discovery. Open-SESAME and Instruct-ERIC workshop: "Remote X-ray Data Collection from European Synchrotrons at the Weizmann Institute of Science" Rehovot, Israel.
- Akanksha Tomar, **Muthusankar Aathi**, Shobhan Kuila, Sharad Vashist, Sheenam Verma, Kottayil. Varughese, Jawahar L. Mehta, Dinakar M. Salunke, Dinakar Sahal, J Jeyakanthan and Arockiasamy Arulandu (2018). Targeting Lectin-like Oxidized-Low Density Lipoprotein (ox-LDL) receptor-1 for Anti-Atherosclerosis Therapy. Council Scientific Advisory, ICGEB, New Delhi, India.
- **Muthusankar Aathi**, Bhaba Krishna Das, Amit Kumar, Shobhan Kuila, Guru Raj Rao R, Jeyakanthan Jeyaraman and Arociasamy Arulandu (2017). Exploring the potential of human dehydroascorbate reductases as novel cancer targets. Annual Symposium of the Indian Biophysical Society, IISER, Mohali, India.
- **Muthusankar Aathi**, Bhaba Krishna Das, Amit Kumar, Guru Raj Rao R, Jeyakanthan Jeyaraman and Arociasamy Arulandu (2017). Molecular Docking Analysis of Small Molecules Targeting Human Chloride Intracellular Channel. ISIN-2017 In-House Symposium of ICGEB, New Delhi, India.
- Akanksha Tomar, **Muthusankar Aathi**, Shobhan Kuila, Sharad Vashist, Sheenam Verma, Kottayil. Varughese, Jawahar L. Mehta, Dinakar M. Salunke, Dinakar Sahal and Arockiasamy Arulandu (2017). Exploring the druggabilty of

LOX-1, a Scavenger Receptor for Oxidized Low-Density Lipoprotein. ISIN-2017 In-House Symposium of ICGEB, New Delhi, India.

- Shobhan Kuila, **Muthusankar Aathi**, Sharad Vashist, Sheenam Verma, Liesel Goveas, Dinakar M Salunke, Dinkar Sahal and Arockiasamy Arulandu (2017). Exploring chloride intracellular channels (CLICs) for anticancer inhibitor discovery. ISIN-2017 In-House Symposium of ICGEB, New Delhi, India.
- **Aathi Muthusankar** and Piramanayagam Shanmughavel (2010). Structural studies on Human NDRG2 protein and their interaction with Natural & Synthetic compounds. A novel drug target for Alzheimer's disease. The Eighth Asia Pacific Conference on Bioinformatics – 2010, Indian Institute of Science, Bangalore, India.

WORKSHOP PARTICIPATED:

- Attended E-workshop "Structure based and ligand based drug design" by JSS college of Pharmacy, Mysuru (2020).
- Hands-on training webinar workshop "Faculty development program on Python" by Indian Institute of Technology, Mumbai (2020).
- Workshop on "Fundamental of Molecular Simulation 2019" by Indian Institute of Technology, Kanpur (2019).
- Hands-on training workshop on "Protein crystallization in lipid bilayer" conducted by ICGEB, New Delhi (2018).

NUCLEOTIDE SEQUENCE SUBMITTED:

- Accession No: JX500416.1
- Accession No: JX500417.1
- Accession No: JX500418.1
- Accession No: JQ687525.1
- Accession No: JQ687526.1
- Accession No: JQ687527.1

THEORTICAL 3D PROTEIN STRUCTURE SUBMITTED:

- Protein Name: SecA ID: PM0077063
- Protein Name: Human NDRG2 Protein ID:PM0078485
- Protein Name: APP ID:PM0080024

- Protein Name: BACE1 ID:PM0080025
- Protein Name: PSEN1 ID:PM0080026
- Protein Name: PSEN2 ID:PM0080027